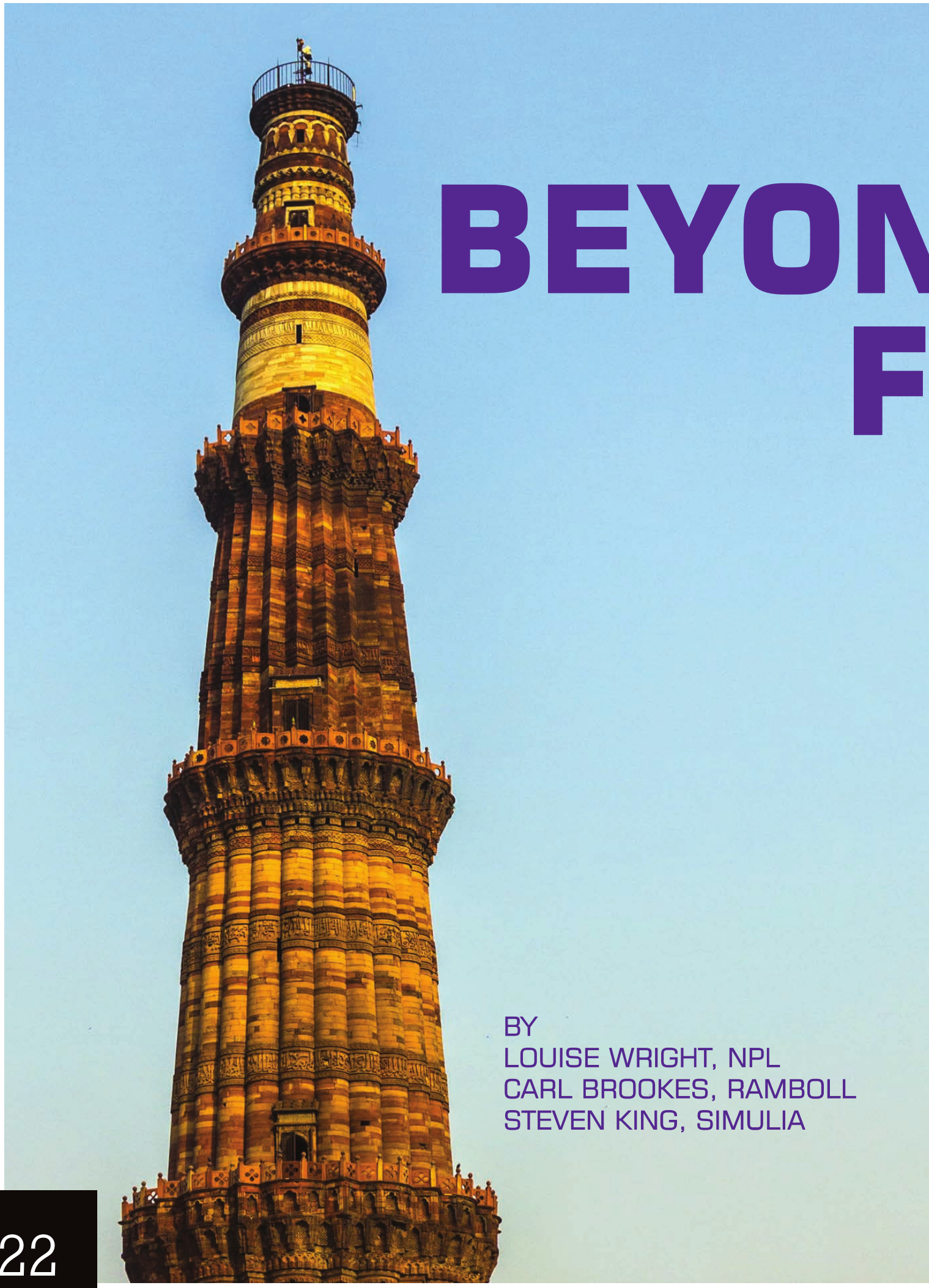

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BY
LOUISE WRIGHT, NPL
CARL BROOKES, RAMBOLL
STEVEN KING, SIMULIA

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CUTTING-EDGE METHODS FOR CHALLENGING PROBLEMS

FE is a well-established technology with a huge range of applications, but "vanilla" FE struggles to solve some classes of problem. Two common classes of problem that are challenging for standard FE are problems involving discontinuities and singularities, such as crack propagation and behaviour at material interfaces, and problems involving large deformations, such as moulding and shaping simulations.

For both classes of problem, careful mesh handling can improve the chances of solving successfully. For instance, the stress singularity at a crack tip can be well-approximated by using second-order elements and shifting the midpoints to be quarter points, and large deformation problems can be approached by stopping the run and remeshing when deformation becomes problematic or by designing an initially deformed mesh that improves with deformation. However, mesh handling is generally time-consuming and requires user expertise. Additionally, there are some problems that mesh handling cannot address. For instance, crack propagation simulation in standard FE restricts the crack growth to a pre-defined path along the element faces, so that only problems where the crack shape is already known can be solved.

Research into methods for solution of challenging problems such as these has developed a range of numerical approaches, and some of the most effective methods have recently been introduced to commercially-available packages. This article discusses how these new methods differ from standard FE, discusses a few of the most established methods, and shows examples of their application to real problems.

What's Different?

We are all familiar with the ideas that underpin FE. An FE model solves a partial differential equation (usually one that defines a physical problem) for some unknown quantity of interest (e.g. displacement, temperature, etc.) by using local numerical approximations defined on a mesh.

The mesh consists of a set of nodes, each of which has one associated basis function, and a set of elements that define how the nodes are linked together. The basis functions, commonly low-order polynomials, are defined on the elements such that the basis function associated with a given node is non-zero only on the elements of which the node is a member. The approximate solution over the whole domain is then written as a weighted sum of the basis functions, where the weights are the values of the unknown quantity at the nodes.

The approximate solution is put into the partial differential equation (PDE) and the associated boundary conditions, which generates a set of simultaneous equations that are solved to obtain the values of the unknown quantity at the nodes, and hence the value of the unknown quantity at any point in the domain.

The new methods typically differ in one of two ways: either they extend the allowable basis functions, or they dispense with the rigid connectivity between nodes that a mesh imposes. Other than these differences, their overall approach is typically similar to that of standard FE. The similarity means that in some cases software routines required for standard FE, such as quadrature routines and routines for solution of simultaneous equations, can also be used, with some adaptations, for solving problems formulated using the new methods.

Enriched finite element methods: XFEM

Methods that extend the allowable basis functions are sometimes known as enriched FE methods or partition of unity methods. Examples include the extended FE method (XFEM), which allows multiple basis functions at a node and will be discussed in more detail below, and hp-adaptive FE, which can associate basis functions with edges, faces, and elements as well as with nodes. The overall approximate solution is still expressed as a weighted sum of the basis functions, but the weights cannot always be associated directly with the value of the unknown quantity at a node.

Enrichment methods are of particular use for problems that have a local feature, with at least approximately understood behaviour, that is of particular importance or interest. A key example is crack propagation. The displacement across a crack and close to the crack tip are comparatively well understood: the displacement across a crack is discontinuous, and the stresses and strains around a crack tip have an r^{-1/2} singularity for a linear

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elastic material. The addition of basis functions that capture this behaviour in the region where the crack is expected to go allows the behaviour to be modelled accurately without mesh refinement.

Each additional basis function has an associated unknown value to be determined by the model, and leads to an additional computational cost incurred by its contributions to the simultaneous equations. However, the extra cost can be minimised by only adding extra functions in the regions that are likely to require enrichment, and in many cases the mesh required for a good solution to be obtained using an

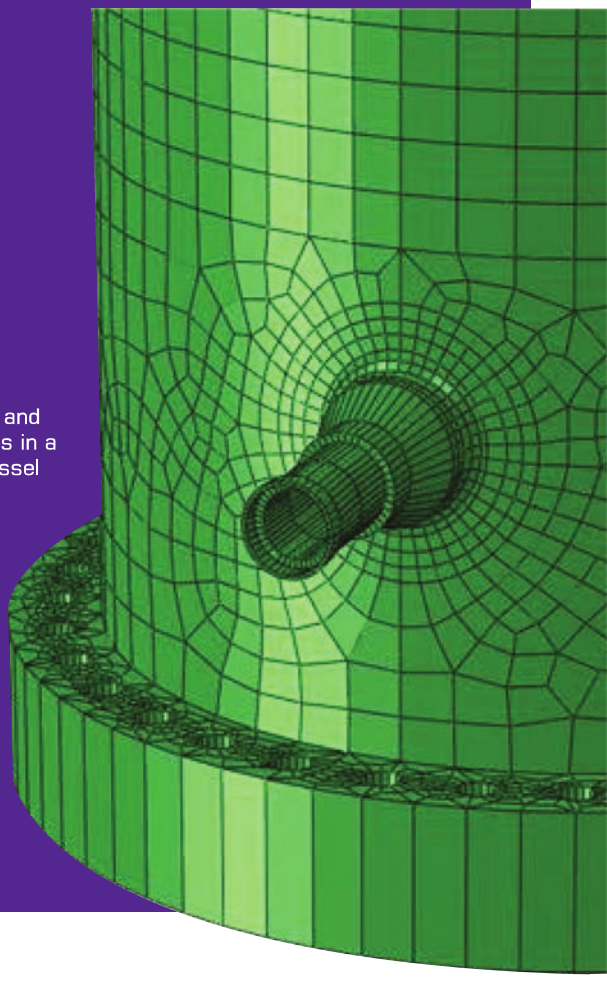


Figure 1:
Model Mesh and Mises Stress in a Pressure Vessel

enriched method will be coarser than the mesh required for an equivalent quality solution using standard FE, meaning that the increase in computational cost can be offset by using a less refined mesh.

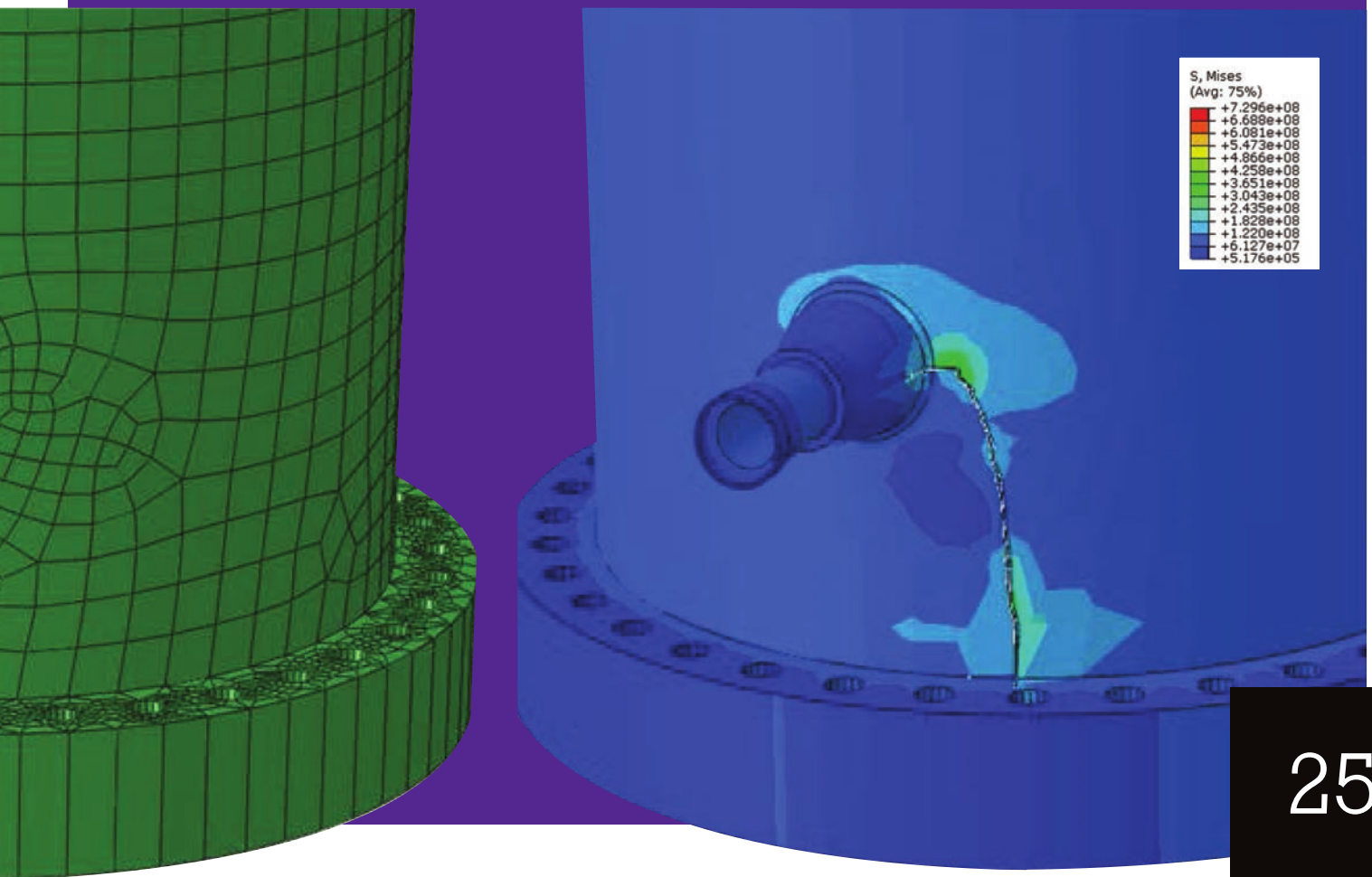
The main enriched method that is seeing an increase in use is XFEM. The development of the method has largely been driven by its suitability for simulation of crack propagation and stress intensity factors, a problem of great importance across a wide range of industries, but other problems also benefit from its local enrichment approach. When applied to crack propagation problems, the XFEM introduces two extra sets of functions in addition to the standard FE nodal basis functions: a step function H(x) to capture the discontinuity in displacement across a crack, and a set of functions Fi(x), typically expressed in polar coordinates centred on the crack tip, that capture the stress singularity in that region. The extra basis functions are defined as the product of these enrichment functions with the standard nodal basis function in order to ensure that the basis functions remain mesh-based and local to the enriched nodes.

The figure above shows the model mesh and the Mises stress in a pressure vessel for a crack initiated in the nozzle where pressure penetration acts on the crack surface. In this case the analysis was allowed to run for 100 increments to allow the crack to extend to the flange. Comparing the mesh and the results shows that the crack does not follow mesh lines, and that the stress and displacement (shown as deformation) are discontinuous across the crack.

Another class of methods that alters the range of basis functions is isogeometric analysis methods. These methods preserve the links between CAD models parameterised by B-splines or NURBS and the model results by using the same three-variable space to parameterise the splines and the FE basis functions, and using tensor products of univariate splines as basis functions. These methods are particularly useful for applications such as contact problems and simulation of turbine blades where the approximation introduced by imposition of a standard FE mesh on the geometry can lead to the loss of important properties such as smoothness or other key geometric details. An additional benefit is that the continuity properties of splines can lead to a reduction in the number of unknown parameters required to obtain a converged result. The main disadvantages of this class of methods are that refinement is challenging, and that creation of a suitable spline or NURBS discretisation via patching can be difficult for problems with complicated topology.

Mesh-free methods

Mesh-free methods, as the name suggests, do not use a mesh to define nodal connectivity. Instead, the basis function associated with a given node is defined in terms of a set of (possibly scaled) coordinates centred on that node. The function is typically defined to be non-zero over some region, sometimes called the “domain of influence”, surrounding the node. A simple choice of domain of influence with potentially useful symmetry properties is a circular region. The basis functions can be chosen to have smoothness properties suitable for



the problem of interest, and can have zero gradient on the edge of the region so that continuity of derivatives is also achieved. Any two nodes whose domains of influence overlap will be linked by one or more of the simultaneous equations.

The linking between nodes can be updated as the solution progresses, ensuring that nodes that are close to one another are linked in the simultaneous equations. Whilst the recalculation of the nodal separations and associated matrix is an additional computational expense, it is usually cheaper than stopping the calculation, extracting the deformed geometry, and remeshing. Atomistic models have to take atomic separations into account for similar reasons, and there are various efficient algorithms originally developed for atomistic models that can be used to track and update nodal connections.

A wide range of meshless methods have been developed. The methods differ in their choice of basis function, in the form of the PDE they use to generate the simultaneous equations, and in their stability and smoothness properties. The oldest, and probably the most widely-used, meshless method is smoothed particle hydrodynamics (SPH), but other methods such as the element-free Galerkin method and the material point method are also used.

A related method that has been used in practical applications in the finite/discrete element method (FDEM). This method combines the strengths of FE and discrete element methods to solve transient dynamic problems that involve multiple deformable bodies interacting.

Discrete element methods simulate discontinuous systems consisting of a (typically large) number of particles, such as powder and granular flows and geomechanics. Each particle generally has displacement and rotational degrees of freedom, can be anything from a point to a polyhedron in shape, and interacts with the other particles via contact and possibly attractive potentials such as cohesion and adhesion. The methods have many similarities to some molecular dynamics modelling methods, particularly since in both cases the key to efficient computation is an effective way of identifying which pairs of particles are likely to interact and ignoring interactions between particles that are too separated to be important.

> “...the extra cost can be minimised by only adding extra functions in the regions that are likely to require enrichment...”

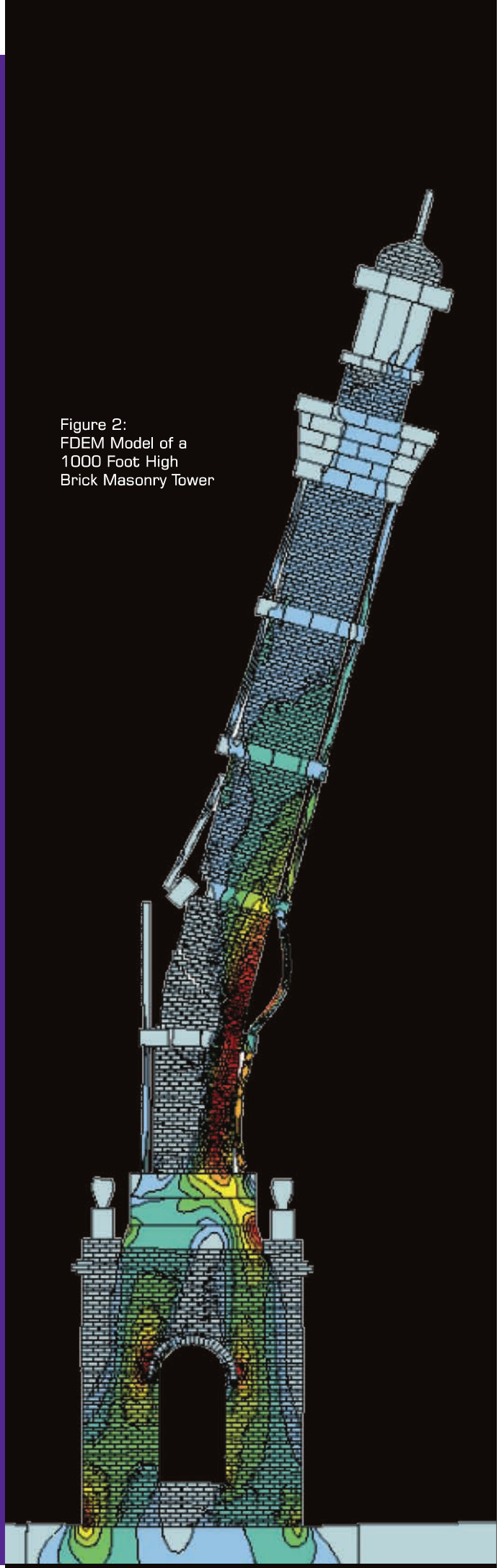


Figure 2:
FDEM Model of a 1000 Foot High Brick Masonry Tower

> “The oldest, and probably the most widely-used, meshless method is smoothed particle hydrodynamics...”

FDEM extends the standard discrete element method by allowing the particles to deform, simulating the deformation using FE techniques. This approach makes it possible to simulate the loading, deformation, and eventual failure, collapse and post-collapse behaviour of inhomogeneous objects such as masonry structures. The technique requires explicit time integration and generally requires a very small time-step for stability, but the use of explicit integration means that the computationally expensive step of matrix inversion, required for implicit time integration, can be avoided.

An example of an area where the use of FDEM has led to a step change in simulation capability is the modelling of masonry bridges. Masonry is a non-homogenised material that undergoes softening and load redistribution as it deforms. Masonry structures can be considered as consisting of a set of interacting deformable units, and hence is ideally suited to simulation with FDEM.

The simulation defines a set of “particles”, typically consisting of a small number of bricks and the associated mortar, and meshes each particle with finite elements. The material properties for these elements are commonly available. The behaviour of the mortar joining the particles together is included by definition of an interface material model that ensures that the contact interaction describes the tension, compression, and friction properties of the mortar correctly.

The Figure 2 shows a FDEM model of a 1000 foot high brick masonry tower. The tower was proposed in the latter part of the nineteenth century but was never built. The simulation here was used to show that had it been constructed it is likely that the foundations would have failed and the tower would have collapsed. By correctly representing the contact interaction between the brick particles, as well as their compressive strength, a realistic simulation of the collapse mechanism was produced. A far lighter and more efficient tower in iron was eventually erected by Eiffel.....

For more on these topics, see:

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